Benzene, 1,4-bis(methylthiomethyl)-

Inchi: InChI=1S/C10H14S2/c1-11-7-9-3-5-10(6-4-9)8-12-2/h3-6H,7-8H2,1-2H3
InchiKey: RXSOGQQIXHXMGS-UHFFFAOYSA-N
Formula: C10H14S2
SMILES: CSCc1ccc(CSC)cc1
Mol. weight [g/mol]: 198.35
CAS: 75919-81-2

Physical Properties

Property code	Value	Unit	Source
gf	202.34	kJ/mol	Joback Method
hf	59.07	kJ/mol	Joback Method
hfus	23.57	kJ/mol	Joback Method
hvap	54.43	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.413		Crippen Method
mcvol	160.700	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
tb	597.42	K	Joback Method
tc	844.95	K	Joback Method
tf	310.20	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.02	J/mol×K	597.42	Joback Method
cpg	376.11	J/mol×K	638.68	Joback Method
cpg	390.18	J/mol×K	679.93	Joback Method
cpg	403.24	J/mol×K	721.19	Joback Method
cpg	415.31	J/mol×K	762.44	Joback Method
cpg	426.43	J/mol×K	803.70	Joback Method
cpg	436.61	J/mol×K	844.95	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75919812&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume